Ballistic thermal rectification

Lifa Zhang,[1] Jian-Sheng Wang,[1] and Baowen Li[1, 2, *]

[1]*Department of Physics and Centre for Computational Science and Engineering, National University of Singapore, Singapore 117542, Republic of Singapore*

[2]*NUS Graduate School for Integrative Sciences and Engineering, Singapore 117456, Republic of Singapore*

(Dated: 8 Feb 2010)

We study ballistic thermal transport in three-terminal atomic nano-junctions by the nonequilibrium Green's function method. We find that there is ballistic thermal rectification in asymmetric three-terminal structures because of the incoherent phonon scattering from the control terminal. With spin-phonon interaction, we also find the ballistic thermal rectification even in symmetric three-terminal paramagnetic structures.

PACS numbers: 05.60.-k, 44.10.+i, 66.70.-f

Introduction Phononics, the study of information processing and controlling of heat flow by phonons, is an emerging new field that is attracting increasing attention [1]. Specifically, researchers have recently modeled and built thermal rectifiers [2], thermal transistors [3], thermal logical gates [4], and thermal memory [5], which are the basic components of functional thermal devices. The most fundamental phononic component is the thermal rectifier – a device that allows larger conduction in one direction than in the opposite direction when it is driven far enough from equilibrium. The effect of thermal rectification is well known to be realized by combining the system inherent anharmonicity with structural asymmetry [2–9]. Whether the rectification can happen in harmonic systems, that is, ballistic rectification, is still unknown, although one recent paper [10] discussed it, in which the authors get different heat conductances by exchanging the heat baths with different structures connected to an asymmetric center part, thus the different conductances come from the totally different systems. As we know, the thermal transport in nanoscale materials, which is very promising for thermal devices, can be regarded as ballistic because of their small sizes in comparison with the phonon mean free path. Therefore, it is highly desirable to investigate whether the ballistic thermal rectification can be realized in harmonic systems, and to explore the necessary conditions for thermal rectification.

The ballistic thermal transport in two-terminal junctions can be described by the Landauer formula. Since the temperatures enter only through the Bose distribution, it is obvious that if we reverse the heat bath temperatures, the heat flux only changes sign, and no rectification is expected. How about the ballistic thermal transport in multiple-terminal junctions? The theory for multiple-terminal electric transport was proposed as the Landauer-Büttiker conductance formula [11–13], and was applied to thermal transport recently [14–16]. From the electronic transport in three-terminal system [13], we know that the third terminal can introduce incoherence or phase breaking to the transport. So it is our interest to investigate whether a multiple-terminal junction is a proper option for ballistic thermal transport, that is, whether the incoherence through the third terminal can induce rectification effect. We will take the nonequilibrium Green's function (NEGF) approach [8, 17–19]. NEGF is widely applied to electronic and thermal transport, and is successful to study the spin Hall effect and phonon Hall effect in junctions [16, 20].

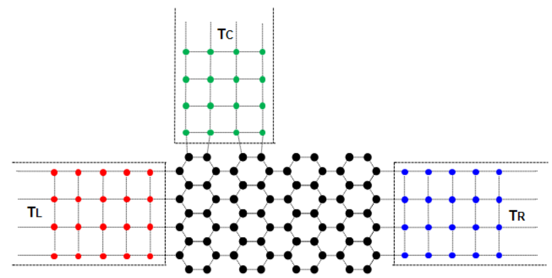

FIG. 1: (Color online) The three-terminal junction setup to study the ballistic thermal transport. The left and right leads have temperatures T_L and T_R, the control terminal lead is adjusted to be T_C or $T_C^{'}$ so that the heat flux from this lead is zero in the forward ($T_L = T_+$, $T_R = T_-$) or backward ($T_L = T_-$, $T_R = T_+$) process. T_+ and T_- are the temperatures of the hot and cold baths, respectively.

Model and Method We consider the ballistic thermal transport in a three-terminal nano-junction as shown in Fig. 1, where a two-dimensional lattice sample, which is a honeycomb lattice, is connected with three ideal semi-infinite leads. The masses are coupled through nearest neighbors by elastic springs (with longitudinal and transverse force constants). We denote the center lattice as $N_R \times N_C$, N_R, N_C correspond to the number of rows and columns, respectively. The external magnetic field can be perpendicularly applied to this part. We use N_{CL} to denote the number of columns of the control lead and N_{CD} to denote the number of columns deviate from the middle of the center part; if $N_{CD} = 0$, the whole setup is symmetric. In Fig. 1, $N_R = 9$, $N_C = 8$, $N_{CL} = 4$, $N_{CD} = -2$. The Landauer-

Büttiker formula can be expressed as,

$$J_\alpha = \sum_{\beta\neq\alpha} \int_0^\infty \frac{d\omega}{2\pi} \hbar\omega\, \tau_{\beta\alpha}(\omega)\big[n(T_\alpha) - n(T_\beta)\big]. \quad (1)$$

Here, $\tau_{\beta\alpha}$ is the transmission coefficient from the αth bath to the βth bath; and $n(T_\alpha) = (e^{\hbar\omega/k_B T_\alpha} - 1)^{-1}$ is the Bose distribution with T_α being the temperature of the αth heat bath. We set $\hbar = 1$ and $k_B = 1$ in the following calculation. Therefore, in the forward process, $T_L = T_+$, $T_R = T_-$, we obtain

$$J_+ = \int \frac{\omega d\omega}{2\pi} \big\{\tau_{RL}(\omega)[n(T_+) - n(T_-)] + \tau_{CL}(\omega)[n(T_+) - n(T_C)]\big\} \quad (2)$$

$$J_C = \int \frac{\omega d\omega}{2\pi} \big\{\tau_{LC}(\omega)[n(T_C) - n(T_+)] + \tau_{RC}(\omega)[n(T_C) - n(T_-)]\big\} \quad (3)$$

Similarly we can obtain the heat fluxes J_- and $J_C^{'}$ in the backward process $T_L = T_-$, $T_R = T_+$. From the equations of $J_C = 0$ and $J_C^{'} = 0$ we can obtain the temperatures of the control bath T_C and $T_C^{'}$; inserting them to the formulae of J_+ and J_-, by the definition of rectification as

$$R = (J_+ - J_-)/\max\{J_+, J_-\}, \quad (4)$$

we can calculate the rectification of this model. If the system is in the linear response regime or in the classic limit, the heat flux from the αth lead can be expressed as $J_\alpha = \sum_{\beta\neq\alpha} \sigma_{\beta\alpha}(T_\alpha - T_\beta)$, we set $T_+ = T_0 + \Delta$, $T_- = T_0 - \Delta$, $T_C = T_0 + \delta$, $T_C^{'} = T_0 + \delta^{'}$, then we obtain

$$\delta = -\delta' = \frac{\sigma_{LC} - \sigma_{RC}}{\sigma_{LC} + \sigma_{RC}}\Delta; \quad (5)$$

$$J_+ = J_- = 2\Delta\left(\sigma_{RL} + \frac{\sigma_{CL}\sigma_{RC}}{\sigma_{LC} + \sigma_{RC}}\right). \quad (6)$$

So there is no rectification in the linear response regime or in the classic limit. In order to get thermal rectification, we should consider the quantum regime out of linear response, and the key work is to compute the transmission coefficients among the heat baths.

In this paper, in addition to the structural asymmetry, we also can introduce the same spin-phonon interaction as in Refs. [16, 22–24] in order to break a time-reversal symmetry. The Hamiltonian of our model can be written as

$$H = \sum_{\alpha=0,L,R,C} H_\alpha + \sum_{\beta=L,R,C} U_\beta^T V_{\beta,0} U_0 + U_0^T A P_0, \quad (7)$$

where $H_\alpha = \frac{1}{2}\left(P_\alpha^T P_\alpha + U_\alpha^T K_\alpha U_\alpha\right)$. The superscript T denotes matrix transpose. Here, $0, L, R, C$ correspond to the center region, left, right, and control leads, respectively. U_α is a column vector for mass reduced displacements in region α, P_α is the associated conjugate momentum vector, and K_α is the force constant matrix, $V_{\beta,0} = (V_{0,\beta})^T$ is the coupling matrix between the βth lead and the central region. A is a block diagonal matrix with diagonal elements $\begin{pmatrix} 0 & h \\ -h & 0 \end{pmatrix}$. h is a model parameter which is supposed to be proportional to the magnetic field. In the first part of this paper, we set $h = 0$; it is a standard harmonic phononic system.

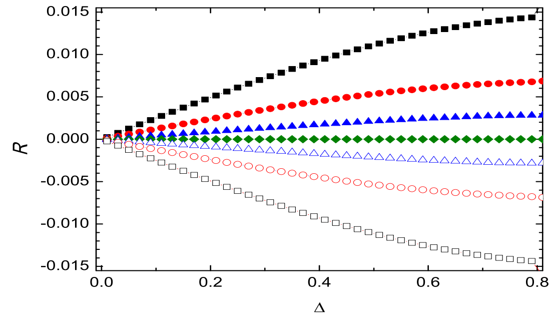

FIG. 2: (Color online) Rectification as a function of relative temperature difference of the hot and cold heat baths. The parameter of the setup is $N_R = 9$, $N_C = 16$, $N_{CL} = 2$. The temperature of the heat bath are $T_+ = T_0(1 + \Delta)$ and $T_- = T_0(1-\Delta)$, where $T_0 = 0.2$ is the mean temperature. The solid square, solid circle, solid triangle, diamond, hollow triangle, hollow circle, hollow square correspond to $N_{CD} = -7$, -5, -3, 0, 3, 5 and 7, respectively.

The retarded Green's function for the central region in frequency domain is [16]

$$G^r[\omega] = \Big[(\omega + i\eta)^2 - K_0 - \Sigma^r[\omega] - A^2 + 2i\omega A\Big]^{-1}. \quad (8)$$

Here, $\Sigma^r = \sum_{\beta=L,C,R} \Sigma_\beta^r$, and $\Sigma_\beta^r = V_{0,\beta} g_\beta^r V_{\beta,0}$ is the self-energy due to interaction with the heat baths, $g_\beta^r = [(\omega + i\eta)^2 - K_\beta]^{-1}$. η is an infinitesimal real positive quantity. The surface Green's functions of the leads g_β^r are obtained following the algorithms of Ref. [18]. The transmission coefficient is

$$\tau_{\beta\alpha}[\omega] = \mathrm{Tr}(G^r \Gamma_\beta G^a \Gamma_\alpha), \quad (9)$$

where, $\Gamma_\alpha = i\big(\Sigma_\alpha^r[\omega] - \Sigma_\alpha^a[\omega]\big)$, $G^a = (G^r)^\dagger$, and $\Sigma_\alpha^a = (\Sigma_\alpha^r)^\dagger$.

Results and Discussions Firstly, we consider the ballistic thermal transport in an asymmetric structure without an external magnetic field. In the following simulation, we set the longitudinal spring constant $k_L = 1.0$, and the transverse one $k_T = 0.25$. If the control lead is connected to the middle of upper edge of the center, that is, $N_{CD} = 0$, the forward process and backward one are exactly the same; no rectification will be expected, as shown in Fig. 2 (the diamond symbols). We will obtain the same result of no rectification if we replace the center honeycomb lattice with the square lattice same as the leads, when the whole system is symmetric wherever

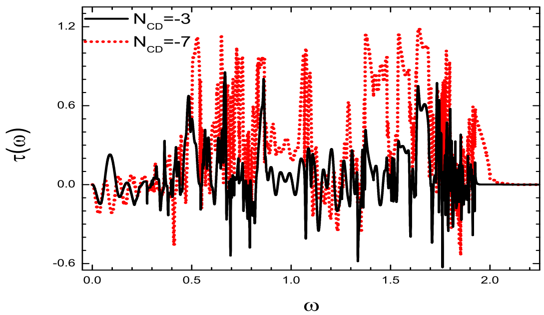

FIG. 3: (Color online) The difference of transmission coefficients: $\tau_{LC} - \tau_{RC}$, as a function of frequency. The parameter of the setup is $N_R = 9$, $N_C = 16$, $N_{CL} = 2$. The solid, dot curves correspond to $N_{CD} = -3$ and $N_{CD} = -7$, respectively.
.

we put the control lead. If the control lead moves away from the center, the rectification effect appears. When the lead is moved the same distance to the left or right, the rectification coefficient has the same magnitude but opposite sign, which is because that the two cases only exchange the value of J_+ and J_-. If the distance between the control lead and the middle of the center part is longer, the rectification effect is larger. In Fig. 2, we can see that the case of $N_{CD} = \pm 7$, when the control lead is next to left or right lead, has biggest rectification. The rectification increases with the temperature difference at far-from-linear-response regime.

From the above formulae, we find if the transmissions τ_{LC} and τ_{RC} are linearly dependent (here $\tau_{\alpha\beta} = \tau_{\beta\alpha}$ because of time reversal symmetry), the rectification will be zero. Figure 3 shows that the transmission coefficients τ_{LC} and τ_{RC} are not linearly dependent, so that the rectification is nonzero. In some frequency domains, $\tau_{LC} > \tau_{RC}$; and in other frequency domains, $\tau_{LC} < \tau_{RC}$. With the distance increasing, that is, from $N_{CD} = -3$ to $N_{CD} = -7$, the difference of τ_{LC} and τ_{RC} enlarges in most part of the whole frequency domain; so that the rectification coefficient increases. Because of scattering from the third bath – the control lead, the total thermal transport from the left lead to the right one is partially incoherent. This phonon incoherence induces rectification. In the whole system the Hamiltonian is quadratic, that is, there is no nonlinearity or anharmonicity, but we still can obtain rectification. Therefore, the phonon incoherence, which can be induced by either nonlinearity or scattering lead, is the necessary condition for thermal rectification.

The control lead acts as a scattering source, which makes the phonon transport incoherent, so that the rectification comes out. However, the width of the control lead does not quite affect the whole thermal transport, which is shown in Fig. 4(a). We make the control lead next to the left lead, and find that the rectification changes little when we increase the width of the lead. If

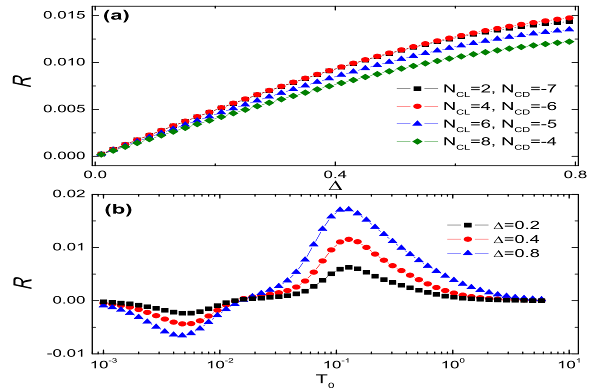

FIG. 4: (Color online) (a) Thermal rectification as function of relative temperature difference Δ for different width of control lead, at $T_0 = 0.2$; (b) Thermal rectification as function of mean temperature for different relative temperature difference. $N_{CL} = 2$, $N_{CD} = -7$. For both (a) and (b), $N_R = 9, N_C = 16$, $T_+ = T_0(1+\Delta)$ and $T_- = T_0(1-\Delta)$.

the width of control lead increases further, the rectification decreases because the asymmetry decreases. Figure 4(b) shows the rectification dependence on temperature, and reproduce the reversal of rectification found in Ref. [9]. At a low temperature, the contribution to thermal transport only comes from the low frequency phonons; if the temperature increases, more high frequency phonons will contribute to the heat transport. From Fig. 3, the relations between transmissions τ_{LC} and τ_{RC} in low frequency domain and high frequency domain are opposite, so that the rectification reverses with the temperature increasing. When the temperature increases further, the system will go to the classic limit, the rectification disappears.

From the previous work [2, 6, 21] on thermal rectification, we know that in order to get rectification, we need

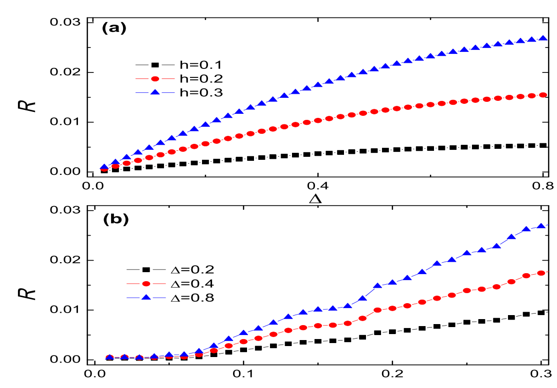

FIG. 5: (Color online) (a) Thermal rectification as function of relative temperature difference Δ for different external magnetic fields. (b) Thermal rectification as a function of magnetic field h. For both (a) and (b): $N_R = 9$, $N_C = 16$, $N_{CL} = 2$, $N_{CD} = 0$. $T_+ = T_0(1+\Delta)$, $T_- = T_0(1-\Delta)$. T_0=0.2.

the structural asymmetry. However, in the nanoscale rectifier, it is not easy to control the structural asymmetry or not easily distinguish the rectification direction by the structural asymmetry. Is there any other means to introduce asymmetry to induce rectification? From the study of phonon Hall effect [16, 22–24], it is known that the magnetic field can influence the thermal transport by the spin-phonon interaction. Thus the magnetic field can break the symmetry of the phonon transport. We apply an external magnetic field perpendicular to the center part of a symmetric structure to study the ballistic thermal transport, the results are shown in Fig. 5. The thermal rectification effect as a function of the temperature difference is shown in Fig. 5(a). R increases with the temperature difference, and can be about 3% if $\Delta = 0.8$ and $h = 0.3$ at $T_0 = 0.2$. Figure 5(b) shows that the rectification can monotonically increase with the external magnetic field in the range of $h = 0 \sim 0.3$. The applied magnetic field breaks the symmetry of the phonon transport system through the spin-phonon interaction, so the transmission coefficient from the control lead to left one is different from that to right one. Figure 6 shows that the two transmission coefficients are not linearly dependent; and with the increasing of magnetic field, the difference of these two transmissions will enlarge, which induce bigger rectification effect. Here all quantities are dimensionless, if we use the parameters for real materials, the rectification coefficient may be different, but would be likely in the range of few per cents.

Although all our values for rectification are small, if we can devise a chain of such ballistic rectifiers, the total rectification can be as large as we need. Because for most nanoscale materials the thermal transport is ballistic and temperature can be applied far from linear response regime, our prediction can be tested by experiments. The asymmetric quasi-two-dimensional nanostructure of any material can have ballistic thermal rectification, such as a graphene sheet. Or the symmetric structure with spin-obit interaction, such as paramagnetic dielectrics, can also have ballistic rectification applied an perpendicular magnetic field.

Conclusions Using the nonequilibrium Green's function method, we have studied ballistic thermal transport in three-terminal atomic nano-junctions. Adjusting the temperature of the control lead in order to make the heat flux from this lead be zero, we can calculate the thermal rectification effect. In the quantum regime out of linear response, there is ballistic thermal rectification in asymmetric three-terminal structures because of incoherent phonon scattering from the control terminal. Through spin-phonon interaction, we also find the ballistic thermal rectification in symmetric three-terminal paramagnetic structures applied an external magnetic field. Therefore, not the nonlinearity, but the phonon incoherence, which can be induced by nonlinearity or scattering boundary or scattering lead, is the necessary condition for thermal rectification. Another necessary condition is asymmetry, not necessarily being structural asymmetry, which can be introduced by an applied external magnetic field through the spin-phonon interaction.

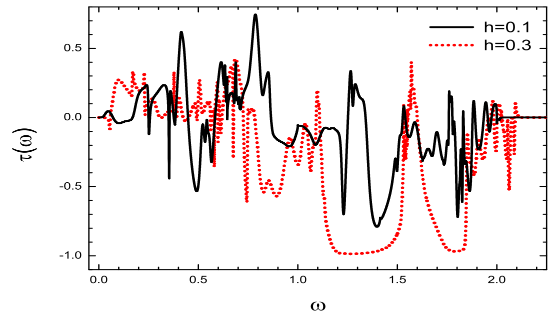

FIG. 6: (Color online) The difference of transmission coefficients: $\tau_{LC} - \tau_{RC}$, as a function of frequency for different applied magnetic fields. The parameter of the setup is $N_R = 9$, $N_C = 16$, $N_{CL} = 2$, $N_{CD} = 0$. The solid, dot curves correspond to $h = 0.1$ and $h = 0.3$, respectively.

Acknowledgements We thank Xiaoxi Ni, Jie Ren and Jie Chen for fruitful discussions. LZ and BL are supported by the grant R-144-000-203-112 from Ministry of Education of Republic of Singapore. JSW acknowledges support from a faculty research grant R-144-000-257-112 of NUS.

* Electronic address: phylibw@nus.edu.sg

[1] L. Wang and B. Li, Physics World **21**, No.**3**, 27 (2008).

[2] B. Li, L. Wang, and G. Casati, Phys. Rev. Lett. **93**, 184301 (2004); B Li, J.-H Lan, L Wang, *ibid* **95**, 104302 (2005); C. W. Chang, D. Okawa, A. Majumdar, and A. Zettl, Science **314**, 1121 (2006). J.-H Lan and B Li, Phys. Rev. B **74**, 214305 (2006).

[3] B. Li, L. Wang, and G. Casati, Appl. Phys. Lett. **88**, 143501 (2006); W. C. Lo, L. Wang, and B. Li, J. Phys. Soc. Jpn. **77**, 054402 (2008).

[4] L. Wang and B. Li, Phys. Rev. Lett. **99**, 177208 (2007).

[5] L. Wang and B. Li, Phys. Rev. Lett. **101**, 267203 (2008).

[6] D. Segal and A. Nitzan, Phys. Rev. Lett. **94**, 034301 (2005).

[7] L.-A. Wu and D. Segal, Phys. Rev. Lett. **102**, 095503 (2009).

[8] T. Ruokola, T. Ojanen, and A. -P. Jauho, Phys. Rev. B **79**, 144306 (2009).

[9] L. Zhang, Y-H Yan, C.-Q Wu, J. -S. Wang, and B. Li, Phys. Rev. B **80**, 172301 (2009).

[10] P. E. Hopkins and J. R. Serrano, Phys. Rev. B **80**, 201408(R) (2009).

[11] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge Univ. Press, 1995).

[12] M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986); M. Büttiker, IBM J. Res. Developm. **32**, 317 (1988); Phys. Rev. B. **38**, 9375(1988).

[13] Y. M. Blanter and M. Büttiker, Phys. Rep. **336**, 1 (2000).

[14] Q. -F. Sun, P. Yang, and H. Guo, Phys. Rev. Lett. **89**,

175901 (2002).

[15] Y. Ming, Z. X. Wang, Q. Li, and Z. J. Ding, Appl. Phys. Lett. **91**, 143508 (2007).

[16] L. Zhang, J. -S. Wang and B. Li, New J. Phys. **11**, 113038 (2009).

[17] H. Haug and A. P. Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, 1996).

[18] J.-S. Wang, J. Wang, and N. Zeng, Phys. Rev. B **74**, 033408 (2006); J.-S. Wang, J. Wang, and J. T. Lü, Eur. Phys. J. B **62**, 381 (2008); L. Zhang, J. -S. Wang and B. Li, Phys. Rev. B **78**, 144416 (2008).

[19] T. Ojanen and A. -P. Jauho, Phys. Rev. Lett. **100**, 155902 (2008)

[20] L. Sheng, D. N. Sheng, and C. S. Ting, Phys. Rev. Lett. **94**, 016602 (2005).

[21] N. Zeng and J.-S. Wang, Phys. Rev. B **78**, 024305 (2008).

[22] L. Sheng, D. N. Sheng, and C. S. Ting, Phys. Rev. Lett. **96**, 155901 (2006).

[23] Yu. Kagan and L. A. Maksimov, Phys. Rev. Lett. **100**, 145902 (2008).

[24] J.-S. Wang and L. Zhang, Phys. Rev. B **80**, 012301 (2009).